



## Systematic Process Design and Operation of Intensified Processes

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# 362191 Systematic Process Design and Operation of Intensified Processes

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Process Intensification (PI) is one of the many options to match current and future challenges of the (bio)chemical industry and it has the potential to improve existing processes as well as new designs of processes to achieve a more sustainable and economic production [1]. However, to date only a few intensified technologies have been implemented in the industry [2, 3] as many issues related to implementation and operations are still not clear. One such issue is the question of controllability and operability of intensified processes. A new approach is to tackle process intensification and controllability issues simultaneously, in the early stages of process design. This simultaneous synthesis approach provides optimal operation and more efficient control of complex intensified systems. Most importantly, it identifies and eliminates potentially promising alternatives but that may have controllability problems later. It may also suggest innovative process solutions which are more economically and environmentally efficient and agile. Note however, due to the integration of functions/operations into one system the controllability region of intensified equipment may become smaller.

In this work, integrated design and operation of intensified operations are considered systematically through a computer-aided framework. To assure that design decisions give the optimum operational and economic performance, operability and controllability issues are considered simultaneously with the process design issues. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions. To demonstrate the application of the computer-aided framework, production of methyl-tert-butyl-ether (MTBE) from methanol and isobutene using a reactive distillation column (RDC) is selected. First, a set of simple design methods for RDC that are easy to use and similar in concept to nonreactive distillation design methods are used. The methods are based on the element concept which is used to translate a ternary system of compounds (methanol, isobutene and MTBE) to a binary system of elements (elements A and B) [4]. For a binary element system, a simple reactive McCabe-Thiele-type method (to determine the number of reactive stages) has been used. The reactive equilibrium curve is constructed through sequential calculation of reactive bubble points. For an energy-efficient design, the driving-force approach (to determine the optimal feed location) for a reactive system has been employed [5]. For both the reactive McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements. ICAS-PDS has been used to compute the reactive vapor-liquid equilibrium data set. It has been shown previously that designing a reactive distillation column at the maximum driving force will result in the minimum energy consumption. Note, that the same principles that apply to a binary compound system are

valid also for a binary element system [6]. Therefore, it is advantageous to employ the element based method for multicomponent reacting systems.

The operation of the RDC is investigated at the highest driving force (point 1) and two other candidate points (points 2 and 3). It is shown analytically and through rigorous dynamic process simulation (using ICAS process simulation software) that the sensitivity of the system to the disturbances in the feed at the highest driving force (point 1) is less than the two other candidate points. By application of this method, the intensified design option is verified to have the inherent ability to reject disturbances resulting in the most self-regulating design. The sustainability and economic metrics are also calculated at points 1, 2 and 3 and it is shown that the operation of RDC at point 1 not only results in an optimal operation, but also in a more economic and environmental friendly design option.

### References:

- [1] P. Lutze, D.K. Babi, J.M. Woodley, R. Gani, 2013. *Ind. Eng. Chem. Res.*, 52, 7127.
- [2] P. Lutze, A. Román-Martinez, J.M. Woodley, R. Gani, 2012. *Compt. Chem. Eng.*, 36, 189.
- [3] S.S. Mansouri, M.I. Ismail, D.K. Babi, L. Simasatitkul, J.K. Huusom, R. Gani, 2013. *Processes*, 1, 168.
- [4] E.S. Pérez-Cisneros, R. Gani, M.L. Mikkelsen, 1997. *Chem. Eng. Sci.*, 52, 527.
- [5] O.S. Daza, E.S. Pérez-Cisneros, E. Bek-Pedersen, R. Gani, 2003. *AIChE J.*, 49, 2822.
- [6] R. Gani, E. Bek-Pedersen, 2000. *AIChE J.*, 46, 1271.

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